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The Development of a Three-Dimensional Partially Elliptic Flow Computer Program for Combustor Research

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SUMMARY

To advance the computational capability for combustor research, a three-dimensional partially elliptic flow computer program is developed from a concept originated by Spalding. Without requiring three-dimensional computer storage locations for all flow variables, the partially elliptic flow program is capable of predicting three-dimensional combustor flow fields with large downstream effects. This program requires only slight increase of computer storage over the parabolic flow program from which it was developed.

A finite-difference formulation for a three-dimensional fully elliptic turbulent reacting flow field is derived. Because of the negligible diffusion effects in the main flow direction in a supersonic combustor, the set of finite-difference equations can be reduced to a partially elliptic form. Only the pressure field is governed by an elliptic equation and requires a three-dimensional storage location in numerical computations. All other dependent variables are governed by parabolic equations similar to those in the parabolic flow program and require only two-dimensional storage locations. A numerical procedure which combines the previously used marching-integration scheme and an iterative scheme for solving the elliptic pressure field is adopted in the present program.

Because of a lack of suitable experimental measurements, calculations were performed to compare with corresponding calculations made using the

parabolic flow program. Comparisons show that physically meaningful differences are predicted. These differences are especially significant in calculations of combustion flow fields. Finally, capabilities and limitations of the present program are discussed and future extensions are suggested.

SYMBOLS

A	expression, eq. (3)
C_1, C_2, C_D	empirical constants associated with the turbulence model
D^u, D^v, D^w	coefficients of pressure gradients in the x,y,z directions, respectively
E	empirical constant, eq. (7)
f	mass fraction
F	expression, eq. (12)
H	total enthalpy
k	turbulence kinetic energy
M	Mach number
p	pressure
Pr	Prandtl number
S	source term, eq. (1)
T	temperature
u,v,w	velocity components in the x,y,z direction, respectively
x,y,z	rectangular coordinates
Γ	exchange coefficeint
δ	distance between two node points
ε	turbulence dissipation energy rate
κ	empirical constant, eq. (7)

μ	viscosity
ρ	density
τ	shear stress
ϕ	general dependent variable, eq. (1).

Subscripts:

eff	effective
e,w,s,n,u,d	east, west, south, north, upstream, downstream faces, respectively.
E,W,S,N,U,D	east, west, south, north, upstream, downstream points, respectively
H_2O	water vapor
j	jet
ℓ	laminar
P	arbitrary node point
t	turbulent
TH	total hydrogen
w	wall
ϕ	general dependent variable

Superscripts:

+	nondimensional variable, eq. (7)
*	guessed or approximate quantity
'	correction variable.

I. INTRODUCTION

A computational approach to the prediction of three-dimensional turbulent reacting flow fields in supersonic combustors along with experimentation has been adopted at NASA Langley Research Center for the scramjet combustor development. Such a computational approach is intended to supplement the traditional, expensive, cut-and-try experimental approach and to help overcome some of the experimental difficulties associated with the scramjet combustor development.

In the computational approach, the computer storage and computing time are always prime concerns in developing a computer program. However, by recognizing special characteristics of the flow field, mathematical and physical simplifications can often be made, so that useful engineering results can be obtained economically within the existing computer capabilities. One such computer program is the SHIP[1] (Supersonic Hydrogen Injection Program) computer program, which has recently been evaluated, improved, and employed for supersonic combustor design at NASA Langley Research Center.[2,3] The SHIP program is based on a set of parabolic three-dimensional flow equations simplified from the full Navier-Stokes equations together with equations for turbulence kinetic energy, dissipation rate, and species concentrations. Because of the parabolic flow simplification, all flow variables require only two-dimensional computer storage and a marching integration procedure can be used in the main flow direction. The main limitations for combustor development are inability to predict recirculation flow fields which occur adjacent to fuel injectors and in separated regions near walls, and to predict the downstream feedback effects due to the presence of embedded subsonic flow fields.

The aforementioned limitations of the SHIP program could be overcome by developing a three-dimensional, fully elliptic flow computer program for the entire combustor. Such a three-dimersional computer program would require a three-dimensional computer storage location for each of more than twenty flow variables. In addition to other mathematical and physical complications, such a fully elliptic approach would be impractical and uneconomical using present computers. Since recirculations are usually localized, they may be either modeled or computed separately from the main combustor flow field. Flow separation close to a wall is associated with energy and total pressure losses in the combustor; such losses should be minimized in a practical design. Since a predominant flow direction is present in the main flow field of a supersonic combustor, (along which the diffusions of mass, momentum, energy, species, etc. can be neglected), the usual parabolic approximation can be applied to simplify the flow equations. However, embedded subsonic combustion regions can be present within the supersonic stream; thus, downstream effects may be felt upstream by means of pressure disturbance propagated through the subsonic fields. The present partially elliptic flow computer program is developed to take such effects into consideration.

The concept of the numerical partially elliptic approach was originated by Spalding.[4] In view of the approximately parabolic nature of the flow field, all flow variables except the pressure are stored only in two-dimensional locations in the computer. Only the pressure, which is governed by an elliptic equation, requires three-dimensional storage. Thus, it is possible to adopt an iterative marching-integration procedure whereby several iterations of the flow field in the predominant flow direction are made. Each iteration uses an improved estimate of the pressure field obtained from the previous iteration.

Iterations are continued until a convergent solution is obtained. Such a numerical procedure, called a partially parabolic procedure by Spalding, was used to compute an incompressible turbulent flow in a two-dimensional curved duct.[4] The upstream propagation of pressure effects, which cannot be calculated by a parabolic procedure, was demonstrated. The computational advantage of such a procedure over a fully elliptic procedure is very great and was illustrated in ref. 5.

The present partially elliptic flow computer program is developed for a three-dimensional, mixed subsonic-supersonic, turbulent, reacting flow in a rectangular parallelepiped. The governing differential equations and their finite-difference formulations are presented in Section II for a three-dimensional fully elliptic flow field. The necessary boundary conditions for three different boundaries are specified. A method of solving these difference equations is briefly discussed. In section III, the finite-difference equations are reduced to a set of partially elliptic equations. The differences between the partially elliptic and the parabolic formulations are discussed, and the advantage in computer storage of a partially elliptic program over a fully elliptic program is pointed out. In section IV, the numerical computation procedures of the present partially-elliptic program are described. In section V, numerical applications of the program are performed. Differences between the calculations of the present program and of the parabolic program from which it was developed are presented. Finally, the capabilities and limitations of the present program are discussed and future extensions are suggested.

II. FORMULATIONS FOR A FULLY ELLIPTIC FLOW FIELD

In this section, a finite-difference formulation for a three-dimensional fully elliptic flow field is derived. Expressions of boundary conditions for three different boundaries are formulated. These formulations could be used to develop a three-dimensional fully elliptic flow computer program. For the present purpose, however, they are reduced for developing a three-dimensional partially elliptic flow computer program.

To be consistent with the geometry of the present configuration of the supersonic combustor, and also with the existing parabolic flow computer program, the formulation is developed based on an Eulerian formulation in a rectangular coordinate system (x,y,z) with the z-axis coinciding with the main flow direction. The flow field is governed approximately by the Navier-Stokes equations together with the equation of state and the species equations. To account for turbulence effects the laminar exchange coefficients are replaced by the corresponding effective exchange coefficients. The turbulence is described by the "k-ε" two-equation turbulence model.[1] Equilibrium chemical reactions are assumed. This assumption is not essential to the problem development; finite-rate reactions with or without unmixedness can be incorporated without any difficulties. Thus the governing equations can be written in the following general form:

$$\frac{\partial}{\partial x}\left(\rho u\phi - \Gamma_\phi \frac{\partial \phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(\rho v\phi - \Gamma_\phi \frac{\partial \phi}{\partial y}\right) + \frac{\partial}{\partial z}\left(\rho w\phi - \Gamma_\phi \frac{\partial \phi}{\partial z}\right) = S_\phi \qquad (1)$$

where ϕ is a general dependent variable, and Γ_ϕ is a general exchange coefficient. When ϕ = 1, u, v, w, H, f, k or ε, equation (1) corresponds, respectively, to the continuity, three components of momentum, energy, concentration, turbulence kinetic energy, or turbulence energy dissipation rate equation. On the left-hand side of equation (1), the first term represents the sum of convection and diffusion in the x-direction, and the second and third terms are those in the y and z directions, respectively. The term S_ϕ on the right-hand side is called the source term which includes all other terms in the differential equation corresponding to ϕ. The appropriate exchange coefficients Γ_ϕ and source terms S_ϕ for each variable ϕ are listed in Table I. The general effective exchange coefficient is composed of two parts, a turbulent and laminar; i.e.

$$\Gamma_\phi = \frac{\mu_{eff}}{Pr_{eff,\phi}} = \frac{\mu_t}{Pr_{t,\phi}} + \frac{\mu_\ell}{Pr_{\ell,\phi}}$$

where $Pr_{t,\phi}$, $Pr_{\ell,\phi}$, μ_t, and μ_ℓ are, respectively, the turbulent and laminar Prandtl numbers and viscosities. The values of Pr_t, Pr_ℓ and the constants C_1 and C_2 in Table I are usually determined empirically (for example, ref. 1).

The numerical formulation is based on a finite-difference form of equation (1). A "staggered" grid system (refs. 6, 7) is used. An arbitrary node point P is surrounded by six neighboring node points denoted by E, W, S, N, U and D for east, west, south, north, upstream, and downstream, respectively, in three directions as shown in figure 1. The rectangular control volume of P

is chosen such that the faces of the control volume are located at the mid-points e, w, s, n, u and d between P and its respective neighboring nodes. All dependent variables except velocity components are stored at node points, velocity components are stored at mid-points between nodes. The projections of a typical control volume in the xy and yz planes and the locations for velocity components stored are shown in figure 2.

By integrating equation (1) over the control volumes a set of difference equations can be obtained. For example, the net flux of convection and diffusion of the general variable ϕ in the x-direction through the control volume can be written as

$$A_e^x (\phi_E - \phi_P) + A_w^x (\phi_W - \phi_P) \tag{2}$$

with

$$A_c^x = (\Delta y)(\Delta z) \quad \frac{\Gamma \phi_E}{\delta x_E} - \frac{(\rho u)_E}{2} \tag{3a}$$

$$A_w^x = (\Delta y)(\Delta z) \quad \frac{\Gamma \phi_W}{\delta x_W} + \frac{(\rho u)_W}{2} \tag{3b}$$

The fluxes of convection and diffusion in the y and z directions can be expressed in a similar manner. When the source term S_ϕ is linearized, the volume integration of the source term becomes

$$S_\phi\,(\Delta x)(\Delta y)(\Delta z) = S_{u,\phi} + S_{p,\phi}\,\phi \tag{4}$$

The resultant finite-difference equation is expressed in the following form:

$$A_p\phi_P = A_e^x\,\phi_E + A_w^x\,\phi_W + A_s^y\,\phi_S + A_n^y\phi_N + A_d^3\,\phi_D + A_u^3\,\phi_U + S_{u,\phi} \tag{5}$$

with

$$A_p = A_e^x + A_w^x + A_s^y + A_n^y + A_d^3 + A_u^3 - S_{p,\phi} \tag{6}$$

The present formulation is made for a flow field in a rectangular parallelepiped. To solve the set of difference equations of form (5), the boundary conditions for all variables ϕ must be specified at all boundaries. In general, each of the six surfaces of the parallelepiped may be either a surface with uniform flow (e.g. freestream), a symmetry boundary, or a solid wall. At the boundary with uniform flow or of symmetry, the uniform or symmetry boundary conditions are specified respectively. For wall boundaries, the variations of flow variables are very steep close to walls. To avoid the use of extremely fine grids near walls, the wall function method is used.[8] Since the present turbulence model is valid for fully turbulent flows, all node points (except those at walls)

must be located in fully turbulent flow. Hence, the near wall points must be far enough from the wall to ensure that the local Reynolds number is sufficiently large. The flow between the near wall points and the wall is assumed to obey the law-of-the-wall. For example, the velocity component w is expressed as

$$w^+ = \frac{1}{\kappa} \ln E y^+ \tag{7}$$

where $w^+ = w/(\tau/\rho)_w^{1/2}$ and $y^+ = y(\tau\rho)_w^{1/2}/\mu_\ell$ or $\rho C_D^{1/2} k^{1/2} \delta/\mu_\ell$ at the near wall points in the present turbulence model. The empirical constants κ, E and C_D are given values of 0.42, 9.0 and 0.09 respectively; δ is the distance of the near point to the wall. Thus the wall boundary condition for each variable, except the turbulence dissipation rate ε, can be formulated in terms of the flux of the variable (at the near wall point) with an appropriate exchange coefficient derived from the law-of-the-wall. The diffusion flux of ε to the wall is difficult to express. Instead of using the flux and an appropriate exchange coefficient, the dissipation rate itself is specified at the near wall point,

$$\varepsilon_{\text{near wall}} = C_D^{3/4} k^{3/2}/\kappa\delta \tag{8}$$

A summary of the wall boundary conditions for all dependent variables ϕ at the near wall points is presented in Table II.

Several computation procedures are available for solving these three-dimensional finite-difference equations. A relaxation procedure used by

Spalding et al[7] has been found to be efficient and successful.[9,10] This procedure involves a guess and correct scheme for the coupling of velocity with pressure[11], a "hybrid" scheme for modifying the coefficients of the difference equations,[12] and a triple sweep line-by-line iterative scheme using a standard tridiagonal matrix algorithm in the x, y and z directions. Details are given in references 7, 9 and 10. It should be pointed out that the solution of the finite-difference equation (5) at an arbitrary point requires solutions at six neighboring points. Therefore, three-dimensional storage locations are required for all variables. Such a large storage requirement combined with present computer capabilities severely limits the number of node points that can be used and is therefore cause for concern in developing a fully-elliptic computer program. In the next section, the finite-difference formulation will be simplified to a set of partially elliptic equations. The computer program based on a partially elliptic formulation requires much less computer storage than a fully elliptic program but only a small increase in storage over that required for a parabolic program.

III. FORMULATIONS FOR A PARTIALLY-ELLIPTIC FLOW FIELD

As discussed in the Introduction, the main flow field in the supersonic combustor possesses a predominant flow direction. The diffusion of mass, momentum, energy, etc. along the flow direction can be neglected as compared with the corresponding convection. The governing equations, except for pressure, can be simplified to a set of parabolic equations. By assuming a (three-dimensional) pressure field, this set of parabolic flow equations can be solved by a marching-integration procedure along the flow direction (assumed to be in the z-direction).[13] The pressure field is generally governed by an elliptic equation and can be solved by an iterative procedure. In this section the finite-difference equations for such a partially elliptic flow field are obtained. The nature of the equations as related to the method of solution is discussed.

Since the flow variables (except pressure) at a streamwise station depend only on quantities at the immediately upstream station (not on those at the downstream stations), slightly different control volumes are chosen for the finite-difference formulation. The projections of a general control volume in the xy and yz planes are shown in figure 3. In the xy (cross-stream) plane, the control volume is exactly the same as that in figure 2, whereas, the yz (streamwise) plane, the upstream and downstream faces of the control volume are located at U and P. By neglecting all diffusion terms in the z-direction in equation (1), and taking volume integrations of equation (1) over the respective control volumes, a set of finite-difference equations is obtained. The continuity equation becomes

$$[(\rho w)_P - (\rho w)_U](\Delta x)(\Delta y) + [(\rho u)_e - (\rho u)_w](\Delta y)(\Delta z)$$

$$+ [(\rho v)_n - (\rho v)_s](\Delta x)(\Delta z) = 0 \tag{9}$$

The general differential equation for ϕ, except three momentum equations, takes the following form,

$$A_p \phi_P = A_e^x \phi_E + A_w^x \phi_W + A_s^y \phi_S + A_n^y \phi_N + S_{u,\phi} + F_U \phi_U \tag{10}$$

with

$$A_p = A_e^x + A_w^x + A_s^y + A_n^y - S_{p,\phi} + F_U \tag{11}$$

Where A_e^x, A_w^x, A_s^y, A_n^y, $S_{u,\phi}$ are the expressions defined in Section II; F_U depends on the mass flux through the upstream face of the control volume,

$$F_U = (\rho w)_U (\Delta x)(\Delta y)/(\Delta z) \tag{12}$$

For the three momentum equations, the difference equations are formulated based on the control volumes of velocity components

$$A_p u_U = A_e^x u_E + A_w^x u_W + A_s^y u_S + A_n^y u_N + S_{u,u} + F_U u_U \tag{13}$$

$$- D^u (p_P - p_W)$$

$$A_p v_P = A_e^x v_E + A_w^x v_W + A_s^y v_S + A_n^y v_N + S_{u,v} + F_U U \qquad (14)$$

$$- D^v (p_P - p_S)$$

$$A_p w_P = A_e^x w_E + A_w^x w_W + A_s^y w_S + A_n^y w_N + S_{u,w} + F_U w_U \qquad (15)$$

$$- D^w (p_D - p_P)$$

where $D^u = (\Delta x)(\Delta y)(\Delta z)/\delta x_w$, $D^v = (\Delta x)(\Delta y)(\Delta z)/\delta y_s$, and $D^w = (\Delta x)(\Delta y)$. When the local Mach number is greater than one, the last term (pressure gradient) in eq. (15) is replaced by $D^w(p_P - p_U)$.

The boundary conditions for all flow variables must be specified at the boundaries parallel to the z-axis. The formulations of these boundary conditions were discussed in Section II. At the upstream boundary all flow variables must be specified; at the downstream boundary, only the pressure is required in the subsonic flow field.

By comparing the finite-difference equations of the partially-elliptic formulation presented above with those of a parabolic flow problem outlined in reference 1 or 13, it is seen that the two formulations are essentially the same. The differences lie mainly in the treatment of the pressure field and the pressure gradient terms in the three momentum equations. For the parabolic flow problem as described in ref. 13, the streamwise pressure gradient is decoupled from the transverse pressure gradients. Since the downstream pressure effects are negligible in parabolic flows, an approximate velocity field is obtained by setting $dp/dz = 0$ or $P_p(x,y) = P_U(x,y)$. The approximate pressure and velocity fields are then corrected using a pressure correction governed by

a two-dimensional (elliptic) equation derived from the continuity equation. Thus the pressure can be treated as though it were like the other variables, independent of downstream quantities.

In the partially-elliptic flow problem the effects of downstream quantities transmitted through the pressure field are important. To determine such flow-fields, an iterative marching-integration procedure is used. An approximate three-dimensional pressure field denoted by p^* is first assumed and later obtained from the previous iteration. The approximate pressure is corrected by a pressure correction p' governed by a three-dimensional elliptic equation derived from the continuity equation (9). The finite-difference form of the pressure correction equation is

$$A_p' p_p' = A_e' p_E + A_w' p_W + A_s' p_S + A_n' p_N + A_D' p_D + A_U' p_U + S_u' \tag{16}$$

where

$$A_p' = A_e' + A_w' + A_s' + A_n' + A_D' + A_U' \tag{17}$$

$$A_{e,w}' = (\Delta y)(\Delta z)\left[(\rho D^u/A_p)_{e,w} \mp \frac{1}{2}\left(u \frac{\partial \rho}{\partial p}\right)_{e,w}\right] \tag{18a}$$

$$A_{s,n}' = (\Delta x)(\Delta z)\left[(\rho D^v/A_p)_{s,n} \mp \frac{1}{2}\left(v \frac{\partial \rho}{\partial p}\right)_{s,n}\right] \tag{18b}$$

$$A_D' = (\Delta x)(\Delta y)\,(\rho D^w/A_p)_P \tag{18c}$$

$$A'_U = (\Delta x)(\Delta y)[(\rho D^w/A_p)_U + (w \frac{\partial \rho}{\partial p})_U] \tag{18d}$$

$$S'_U = [(\rho w)_U - (\rho w)_D](\Delta x)(\Delta y) + [(\rho u)_w - (\rho u)_e](\Delta y)(\Delta z) \tag{19}$$

$$+ [(\rho v)_s - (\rho v)_n](\Delta x)(\Delta z).$$

All variables in eqs. (17)-(19) are calculated based on the approximated flow field (p^*, etc.). Once the pressure correction p' is obtained from eq. (16), the approximate pressure p^* and velocity components (u^*, v^*, w^*) are corrected as follows

$$p = p^* + p' \tag{20}$$

$$u = u^* + (D^u/A_p)^*_w (p'_W - p'_P) \tag{21}$$

$$v = v^* + (D^v/A_p)^*_s (p'_S - p'_P) \tag{22}$$

$$w = w^* + (D^w/A_p)^*_P (p'_P - p'_D) + (\frac{w}{\rho} \frac{\partial \rho}{\partial p})^*_P p'_P \tag{23}$$

This procedure is repeated for each forward step. The details of the calculation procedures will be described in Section IV.

By inspection of the above difference equations, it can be seen that the solutions at a point (except pressure) depend only on solutions at four neighboring points in the xy (cross-stream) plane. The solution in the pressure correction depends on quantities at six neighboring points. Therefore, to solve

these equations, only the pressure and the pressure correction require three-dimensional storage. The other variables require only two-dimensional storage like a parabolic flow program. In comparison with the three-dimensional fully-elliptic formulation presented in Section II, a great saving of computer storage is realized for a three-dimensional computer program based on the partially-elliptic formulation.

IV. COMPUTATION PROCEDURES AND COMPUTER PROGRAM

In this section the numerical procedures for solving the system of three-dimensional, partially-elliptic, finite-difference equations are described. The computer program thus developed is discussed.

The present numerical procedure combines the marching-integration scheme[13] used in the parabolic flow program[1] and the iterative scheme[5] used for solving the elliptic pressure field. The general calculation steps are outlined in the following:

1. The pressure field is first assumed at all three-dimensional storage locations.

2. A marching-integration procedure is initiated which marches through the flow field. In equations (13)-(15), the pressure gradient terms are evaluated from the assumed pressure field, and the coefficients A, source terms $S_{u,\phi}$ and $F_U\phi_U$ for ϕ = u,v,w are evaluated from the upstream conditions. Then the two-dimensional difference equations (13)-(15) are solved by a double-sweep line-by-line iterative scheme using a tridiagonal matrix algorithm.

3. The newly calculated velocity components are checked for mass conservation at all node points in the xy (cross-stream) plane. The unbalance of mass conservation is necessary for calculation of the pressure correction, which is obtained from eq. (16). Since an iterative scheme is used in solving the three-dimensional pressure field, eq. (16) is simplified by setting $p'_U = p'_D = 0$ to save computer storage. Thus, eq. (16) is reduced to a two-dimensional equation, and can be solved by the double-sweep line-by-line iterative scheme.

4. After obtaining the pressure correction, the pressure and velocity components are then corrected by eqs. (20)-(23).

5. Equation (10) for the other variables (e.g. ϕ = k, ε, H, f, etc.) is also solved by the double-sweep line-by-line iterative scheme, so as to provide flowfield quantities appropriate to a new downstream station.

6. The streamwise march is continued until the end of the partially elliptic flow region is reached. By the end of one complete march (iteration), a new three-dimensional pressure field has been obtained.

7. Steps 2, 3, 4, 5, 6 are then repeated until the pressure corrections at all node points become smaller than a prescribed value. On the last iteration, the converged flow variables are printed out.

As discussed in Section IV, except for pressure, the finite-difference formulation for the partially elliptic flow program is essentially the same as for the parabolic flow program. In the numerical procedures just described, steps 2 to 6 within each iteration are similar to those in the parabolic program. Therefore, the parabolic program provides the main part of the present partially elliptic program. The present program considers three-dimensional, turbulent, reacting (equilibrium) flow in a supersonic combustor in the form of a rectangular parallelepiped. Each lateral boundary of the parallelepiped can be either a solid wall, a symmetry boundary, or a surface with a uniform (or free) stream. The wall boundaries are allowed to vary smoothly along the flow direction.

The pressure field in the present program requires three-dimensional storage. Thus the streamwise dimension of the pressure field determines, and also limits, the maximum number of march steps in each iteration. Pressure gradients are evaluated from the assumed pressure field; consideration is also

given as to whether the local flow field is subsonic or supersonic. In the first iterative solution pressure gradients are assumed to be zero; thus the first iterative solution is the parabolic flow solution. The higher order iterative solutions depend on the pressure fields obtained from the previous iterations. To ensure stability of the iterative procedure a pressure (under) relaxation factor is introduced. Since the flow problem is highly nonlinear, good criteria to determine a suitable value for this factor have not been found. At present this factor is determined by numerical experimentation.

V. APPLICATIONS OF THE PROGRAM

In this section applications of the present program are presented. Because of the lack of good quality experimental data, detailed evaluations of the program by comparing with experiments are not possible at the present time. Therefore, results from the present calculations are compared with results from the parabolic program. Such comparisons demonstrate the importance of the effects predicted by the partially-elliptic program. Furthermore, previous evaluation of the parabolic program has already established its accuracies and capabilities; the numerical comparisons between it and the present program infer the usefulness of the present program to supersonic combustor research.

A numerical example was performed for the flow field of a hydrogen jet mixing with a supersonic airstream in a rectangular duct. As shown in figure 4, a slightly subsonic (M_j = 0.99) hydrogen jet with uniform exit conditions, w_j = 1500 m/sec, T_j = 400 K, and p_j = 0.101 MPa, is located at the center of the duct. The ducted airstream at the jet exit plane is also assumed to be uniform with w = 990 m/sec, T = 1700 K, and p = 0.101 MPa (i.e. M = 1.2). The upper and lower walls diverge slightly to allow for shock and Mach waves to develop and interact with the subsonic stream at the center of the duct. Computations were performed for both reacting and nonreacting cases.

Streamwise pressure variations along the centerline of the duct O and at the duct cover C for both partially elliptic and parabolic nonreacting calculations are shown in figure 5. The convergent partially elliptic calculations were obtained after eleven iterations. Note that streamwise marching steps are used on the abscissa in fig. 5 instead of the usual physical distance; the step size used in all present calculations is 0.004 of the duct height. The downstream

pressure effects considered by the partially elliptic program are clearly demonstrated by the comparison. Because the subsonic region is small, the downstream effects change the centerline pressure only about 2 percent. At the duct corner, the downstream effects through the boundary layer are even smaller. Nevertheless, the present partially elliptic program does predict correctly the qualitative physical phenomena.

From the same calculations cross-duct profiles are presented in figures 6a and b of streamwise velocity w, pressure p, and mass fraction of total hydrogen f_{TH} at y = 0 and 0.5 cm along the lines OA and DB in fig. 4 at step 32 (z = 0.468 cm). Because of the small downstream effects, the differences between the two calculations are small and mainly occur in the subsonic jet region (fig. 6a). As expected, there is no effect in the supersonic flow region (fig. 6b).

The streamwise pressure variations along the centerline of the duct O and the duct corner C for reacting calculations are shown in fig. 7. The partially-elliptic results are obtained based on 11 iterations. Because of the combustion of hydrogen, the centerline pressure increases much more abruptly than in the nonreacting case. The large increase in pressure propagates upstream in the partially-elliptic calculation and causes as much as 14% of pressure difference over the parabolic calculation. Again, the difference in pressures at the duct corner is relatively small; however, the pressure variations due to the occurrence of shock and Mach waves are clearly shown.

Figure 8 shows the convergence behavior of the streamwise pressures of the same reacting calculation. The streamwise march has been extended to 80 steps. Results show that the rate of convergence depends on the distance from the jet exit. The solution converges faster close to the jet exit than

downstream; for example, beyond step 75, the centerline pressure has still not reached the convergent solution even after 26 iterations.

The reacting results for cross-stream profiles of the streamwise velocity w and the mass fraction of total hydrogen f_{TH} at y = 0 (line OA in Fig. 4) and at step 32 are presented in fig. 9a. The profiles of the pressure p and the mass fraction of water vapor are shown in fig. 9b. As in the results shown in fig. 7, the partially-elliptic calculations show differences in these profiles over the parabolic calculations, especially the large difference in the water vapor distribution.

Reacting results of cross-stream profiles at y = 0.5 cm (line DB in fig. 4) and at step 32 are presented in figs. 10a and b. At this location, the downstream effects predicted by the partially-elliptic calculation are much smaller than those near the jet centerline.

Cross-stream profiles at step 52 (z = 0.787 cm) are presented in figures 11 and 12. Because of the large pressure increase and wide spreading of the reacting region, the partially elliptic calculation predicts much larger effects than those at step 32. Even away from the centerline, the effects predicted by the partially elliptic calculation are both quantitatively and qualitatively important.

VI. DISCUSSION AND CONCLUSION

To advance the computational capability for combustor research, a three-dimensional partially elliptic flow computer program has been developed. The program is capable of predicting combustion flow-fields with large downstream effects; this was not possible using a parabolic flow computer program. The physical models and numerical schemes of the development of this partially-elliptic flow program have been consistent with those of the parabolic flow program.

Physically, this partially elliptic flow program adopts a "k-ε" two-equation turbulence model and a model of equilibrium reactions among species. Although the application of such an equilibrium reaction model is limited, it is not difficult to incorporate any finite-rate reaction model into the program. Numerically, this program is based on a finite-difference formulation in a "staggered" grid system. A combined central and upwind difference scheme is used in the finite-difference equations which are then solved by a line-by-line iterative scheme using a tridiagonal matrix algorithm.

The main difference between the present partially elliptic flow program and the parabolic flow program is implied by their names. The parabolic flow program is based on a set of parabolic equations with a known (arbitrary) pressure field. The partially elliptic flow program is based on a similar set of parabolic equations; however, the pressure gradients in the momentum equations are evaluated from a three-dimensional pressure solution. Thus an iterative marching-integration procedure is necessary to obtain the three-dimensional pressure field and the other flow variables. With only a small increase in computer storage over the parabolic flow program, the present program is

capable of predicting the downstream effects.

The importance of the present partially elliptic flow program has been demonstrated by the numerical example presented in Section V. The differences between results obtained from the partially elliptic and parabolic calculations are significant especially in the combustion flow field. Moreover, since chemical reactions are strongly pressure dependent, the downstream pressure effects predicted may have important effects on calculations using finite-rate reactions.

The main physical limitation of the partially elliptic program is its inability to predict recirculation flow fields. For a three-dimensional recirculation flow field, a three-dimensional elliptic flow program is required. The finite-difference formulation and method of solution for such an elliptic flow have been presented in Section II. However, the large computer storage requirement has been a major drawback to development of such a computer program.

The future extensions for the present program include the optimal application of the iterative procedure in order to minimize computer time. Since the number of iterations required depends on the assumed pressure field and the relaxation factor, a rational method to estimate a relaxation factor and to obtain stable iterations is more important. Moreover, it also has been noted that the rate of solution convergence decreases along the streamwise direction; i.e. the upstream flow field requires fewer iterations than the downstream. Thus, the present program should be tailored especially to actual needs. Other work related to combustor development should include the incorporation of a finite-rate chemical reaction model to predict realistic combustion flow fields and the development of efficient solution algorithms to save computer storage and computing time.

In conclusion, the present partially elliptic flow program has advanced the computational capability for combustor research. Combustor flow fields with important downstream effects can now be predicted.

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Table I. The Appropriate Exchange Coefficients Γ_ϕ and Source Terms S_ϕ for Variable ϕ

ϕ	Γ_ϕ	S_ϕ
1	0	0
u	μ_{eff}	$-\frac{\partial p}{\partial x} + \frac{\partial}{\partial x}(\mu_{eff}\frac{\partial u}{\partial x}) + \frac{\partial}{\partial y}(\mu_{eff}\frac{\partial v}{\partial x}) + \frac{\partial}{\partial z}(\mu_{eff}\frac{\partial w}{\partial x}) - \frac{2}{3}\frac{\partial}{\partial x}[\mu_{eff}(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z})]$
v	μ_{eff}	$-\frac{\partial p}{\partial y} + \frac{\partial}{\partial x}(\mu_{eff}\frac{\partial u}{\partial y}) + \frac{\partial}{\partial y}(\mu_{eff}\frac{\partial v}{\partial y}) + \frac{\partial}{\partial z}(\mu_{eff}\frac{\partial w}{\partial y}) - \frac{2}{3}\frac{\partial}{\partial y}[\mu_{eff}(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z})]$
w	μ_{eff}	$-\frac{\partial p}{\partial z} + \frac{\partial}{\partial x}(\mu_{eff}\frac{\partial u}{\partial z}) + \frac{\partial}{\partial y}(\mu_{eff}\frac{\partial v}{\partial z}) + \frac{\partial}{\partial z}(\mu_{eff}\frac{\partial w}{\partial z}) - \frac{2}{3}\frac{\partial}{\partial z}[\mu_{eff}\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial y})]$
H	$\frac{\mu_{eff}}{Pr_{eff,H}}$	$\frac{\partial}{\partial x}[\frac{\mu_{eff}}{2}(1 - \frac{1}{Pr_{eff,H}})\frac{\partial}{\partial x}(u^2+v^2+w^2)] + \frac{\partial}{\partial y}[\frac{\mu_{eff}}{2}(1 - \frac{1}{Pr_{eff,H}})\frac{\partial}{\partial y}(u^2+v^2+w^2)]$ $+\frac{\partial}{\partial z}[\frac{\mu_{eff}}{2}(1 - \frac{1}{Pr_{eff,H}})\frac{\partial}{\partial z}(u^2+v^2+w^2)] + \frac{\partial}{\partial x}[\mu_{eff}(u\frac{\partial u}{\partial x} + v\frac{\partial w}{\partial y} + w\frac{\partial u}{\partial z})]$ $+\frac{\partial}{\partial y}[\mu_{eff}(u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + w\frac{\partial v}{\partial z})] + \frac{\partial}{\partial z}[\mu_{eff}(u\frac{\partial w}{\partial x} + v\frac{\partial w}{\partial y} + w\frac{\partial w}{\partial z})]$ $-\frac{2}{3}\frac{\partial}{\partial x}[u\mu_{eff}(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z})] - \frac{2}{3}\frac{\partial}{\partial y}[v\mu_{eff}(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z})]$ $-\frac{2}{3}\frac{\partial}{\partial z}[w\mu_{eff}(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z})]$
k	$\frac{\mu_{eff}}{Pr_{eff,k}}$	$\mu_t G - \rho\varepsilon$

ε	$\frac{\mu_{eff}}{Pr_{eff,\varepsilon}}$	$C_1\mu_t \frac{\varepsilon}{k} G - C_2\rho\varepsilon^2/k$
f	$\frac{\mu_{eff}}{Pr_{eff,f}}$	0

Note: $G = 2[(\frac{\partial u}{\partial x})^2 + (\frac{\partial v}{\partial y})^2 + (\frac{\partial w}{\partial z})^2] + (\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x})^2 + (\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x})^2 + (\frac{\partial x}{\partial z} + \frac{\partial w}{\partial y})^2$

Table II. Wall Boundary Conditions at Near Wall Points

ϕ	$\phi_{\text{near wall}}$	Γ_{ϕ}, near wall	
Velocity components normal to the wall	- (0 at wall)	0	
Velocity components parallel to the wall	- (0 at wall)	$\dfrac{\mu_{\ell} y^{+}}{\frac{1}{\kappa}\ln(Ey^{+})}$	$y^{+} > 11.5$
		μ_{ℓ}	$y^{+} \leq 11.5$
k	- (0 at wall)	0	
ε	$C_D^{3/4} k^{3/2}/\kappa\delta$	-	
f	-	0	
H	-	$\dfrac{\mu_{\ell}}{Pr_{t,H}} \dfrac{y^{+}}{\frac{1}{k}\ell n(Ey^{+}) + P_H}$	$y^{+} > 11.5$
		$\dfrac{\mu_{\ell}}{Pr_{\ell}}$	$y^{+} \leq 11.5$

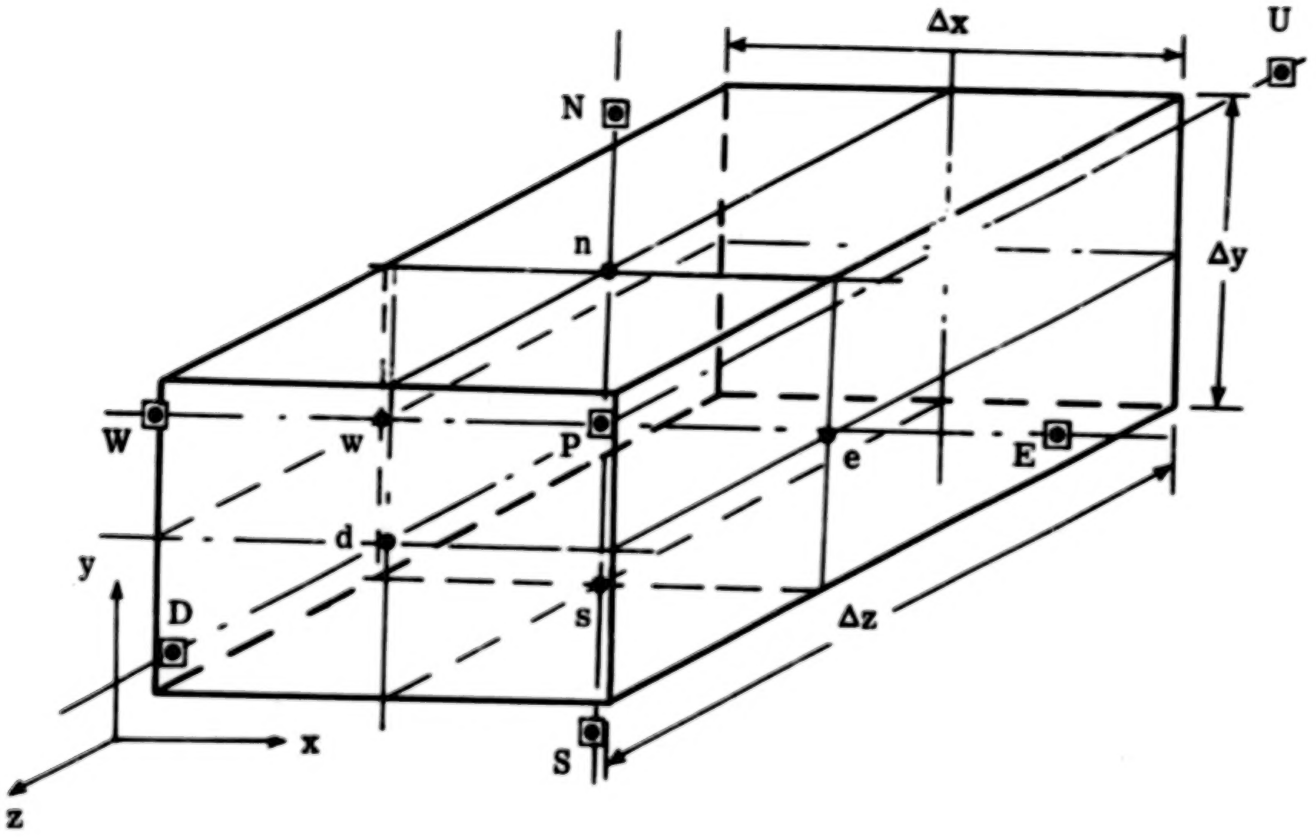

Figure 1.- Grid and control volume for scalar quantities.

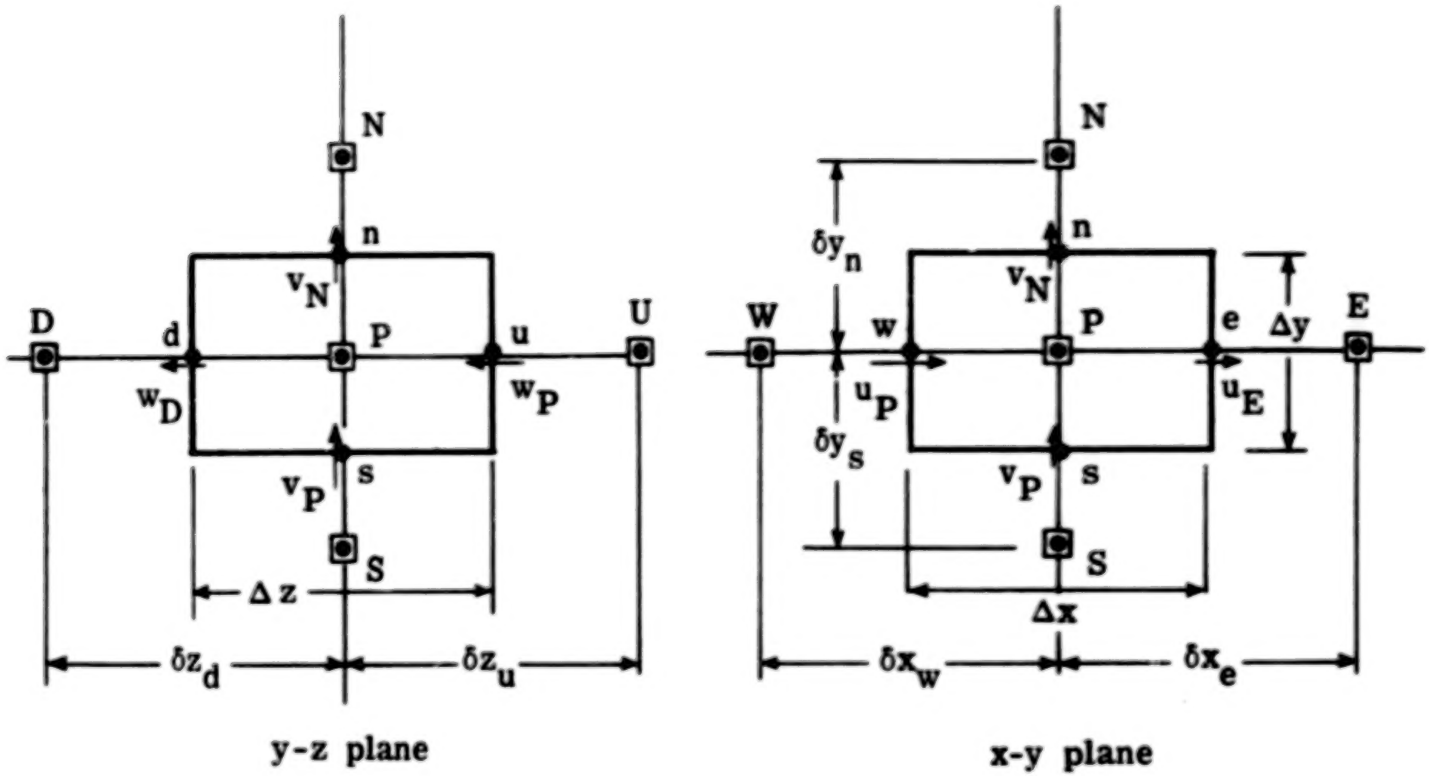

Figure 2.- Projections of the control volume and the storage locations for velocity components.

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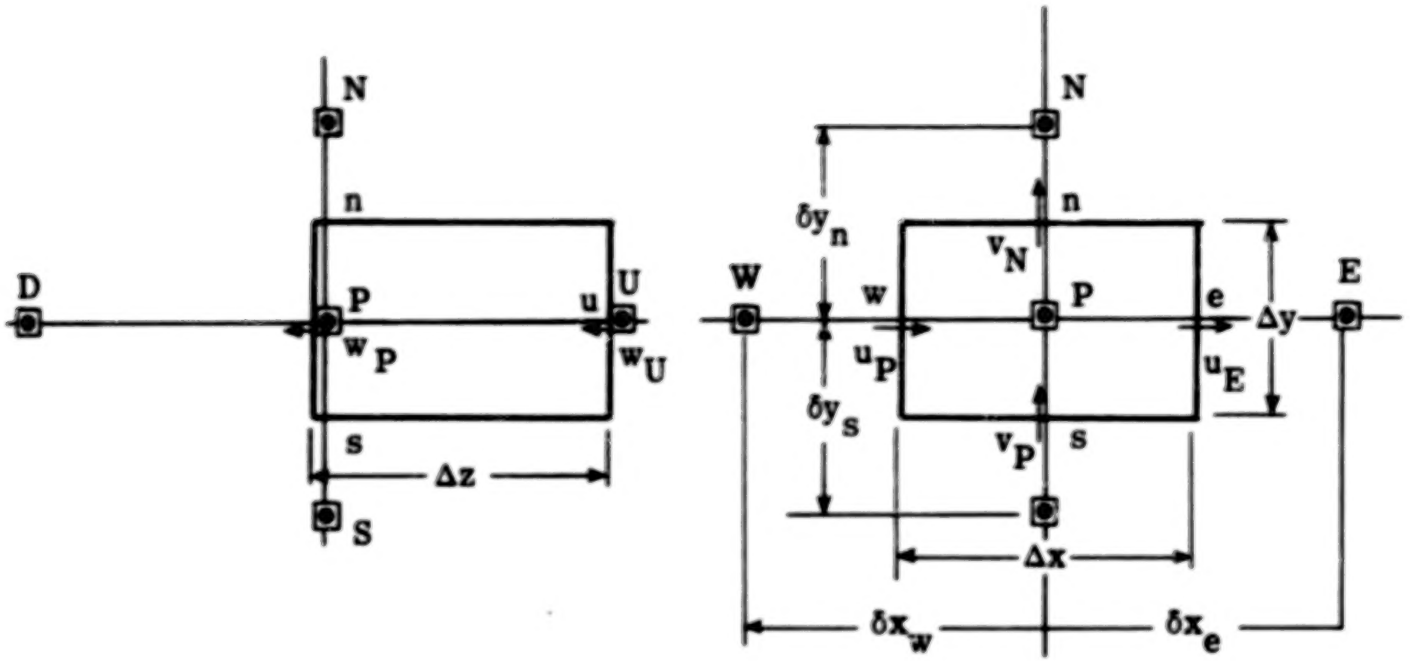


y-z plane

x-y plane

Figure 3.- Projections of the control volume for the partially-elliptic formulation.

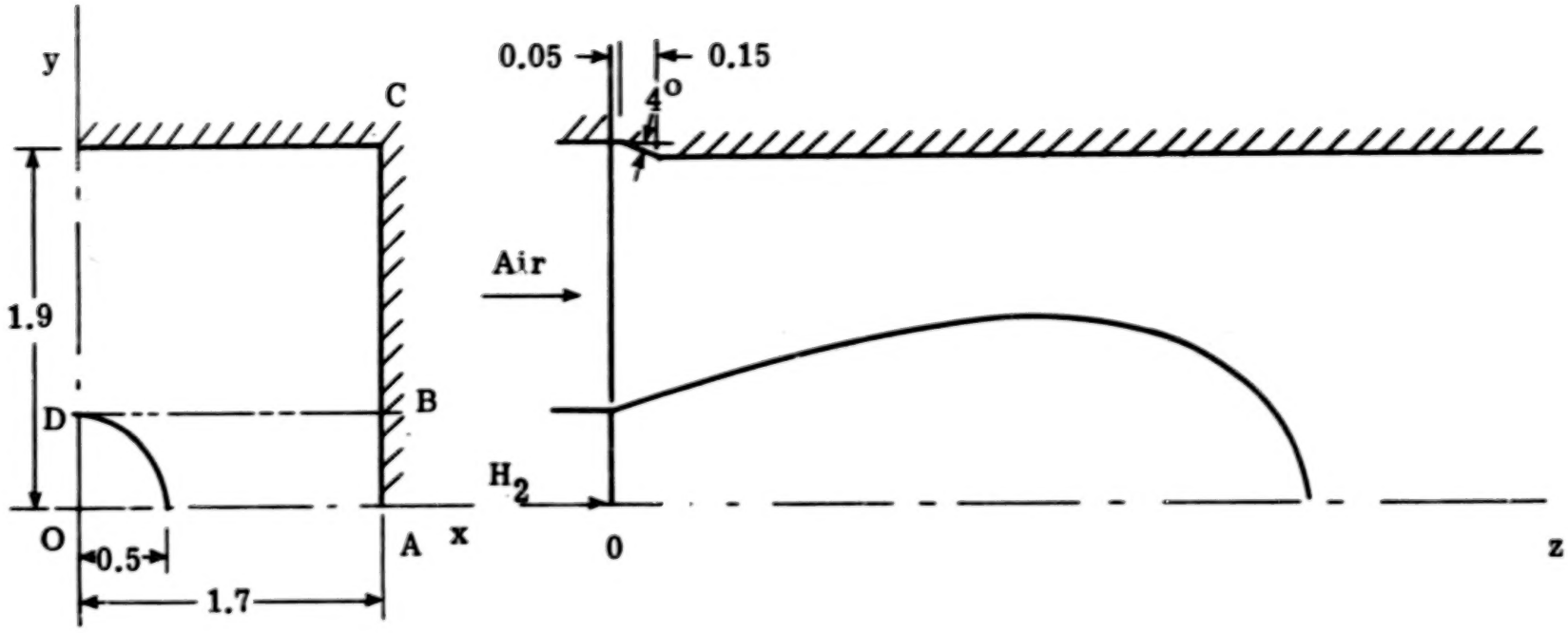


Figure 4.- Mixing of a subsonic hydrogen jet with a ducted supersonic airstream.
(Dimensions are in centimeters)

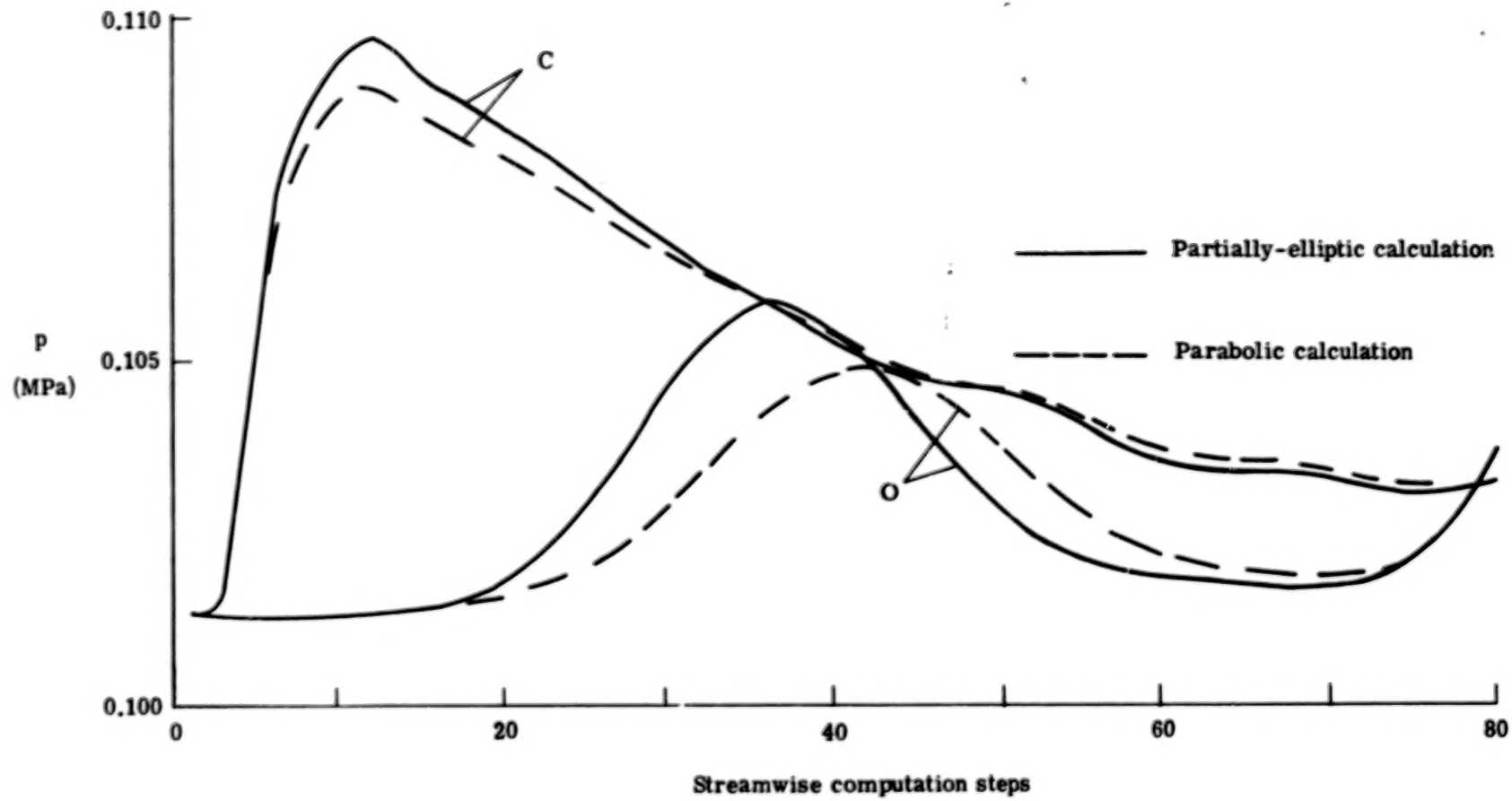
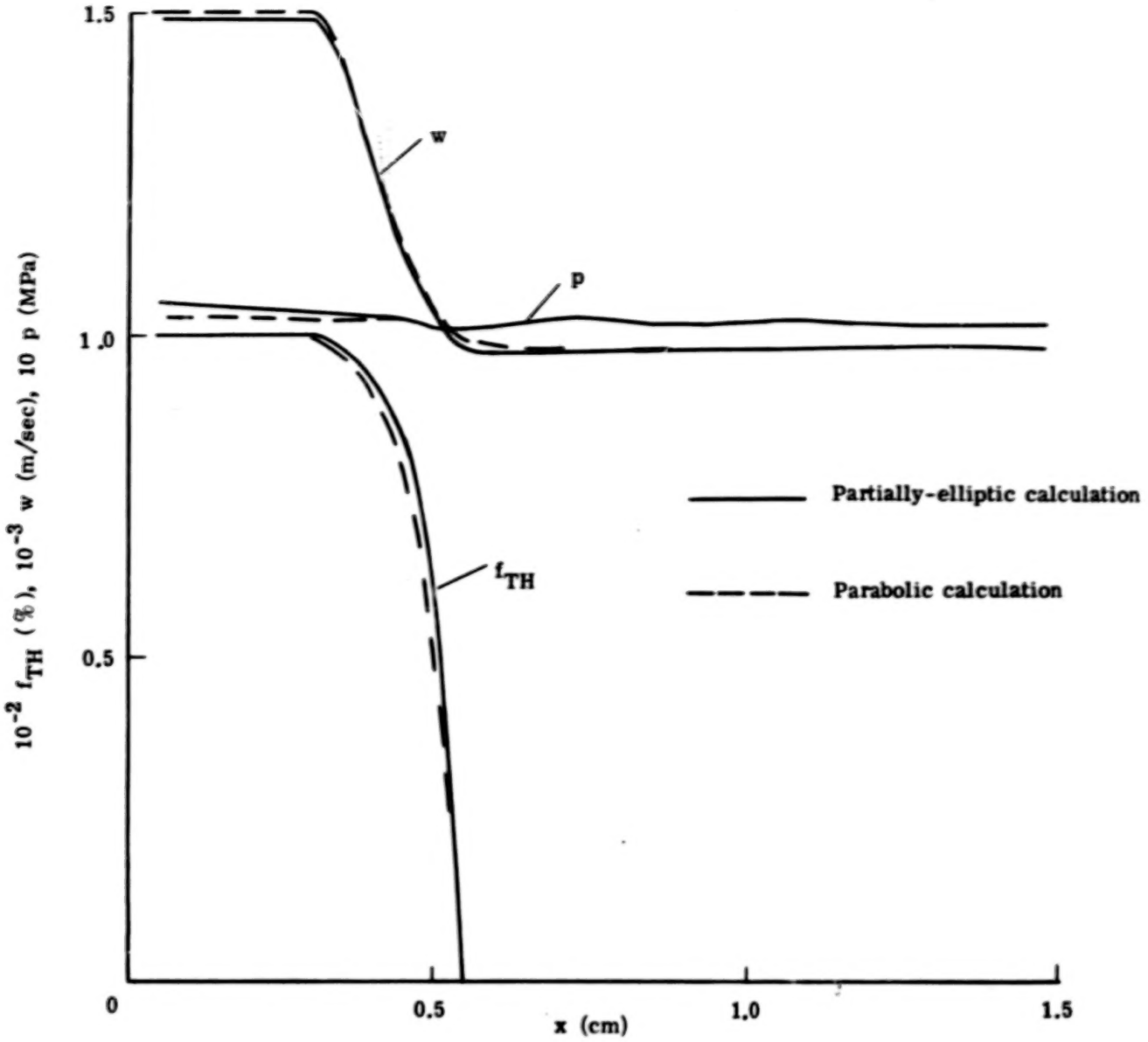
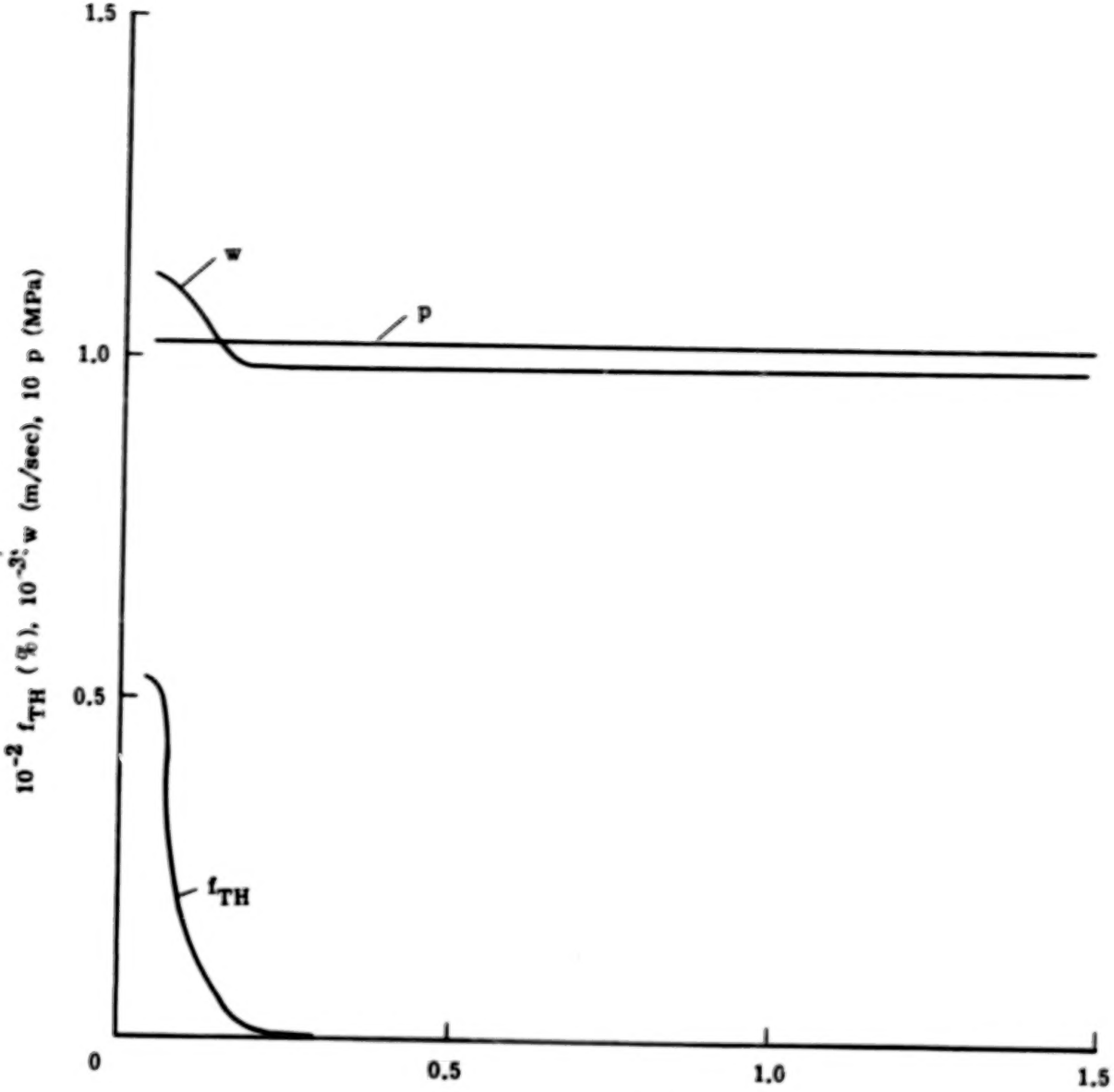


Figure 5.- Streamwise pressure variation along the centerline of the duct and at the duct corner; non-reacting case.



(a) y = 0.

Figure 6.- Cross-duct profiles of velocity, pressure, and mass fraction at step 32 (z=0.468 cm); non-reacting case.



(b) y = 0.5 cm.

Figure 6.- Concluded.

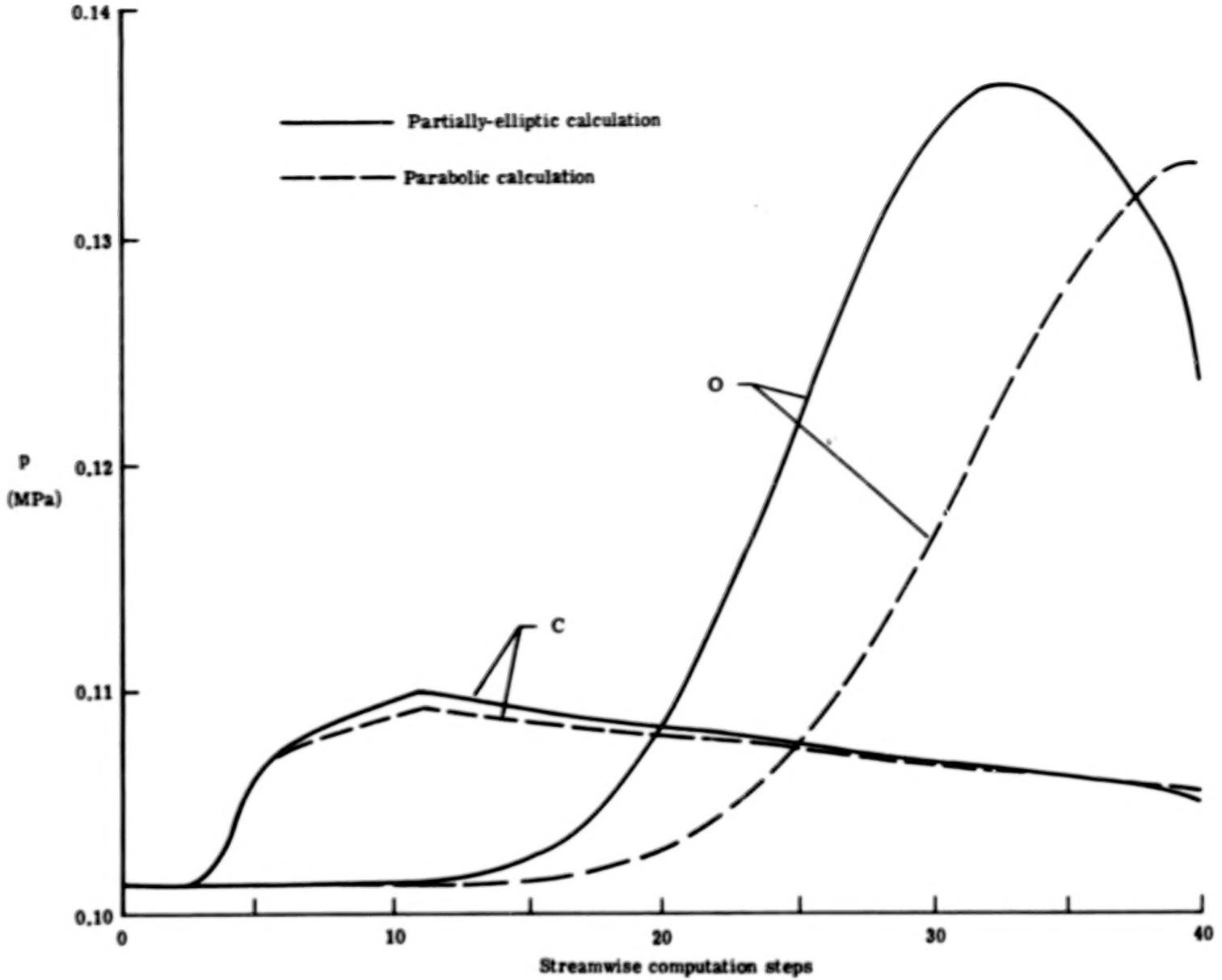


Figure 7.- Streamwise pressure variation along the centerline of the duct and at the duct corner: reacting case.

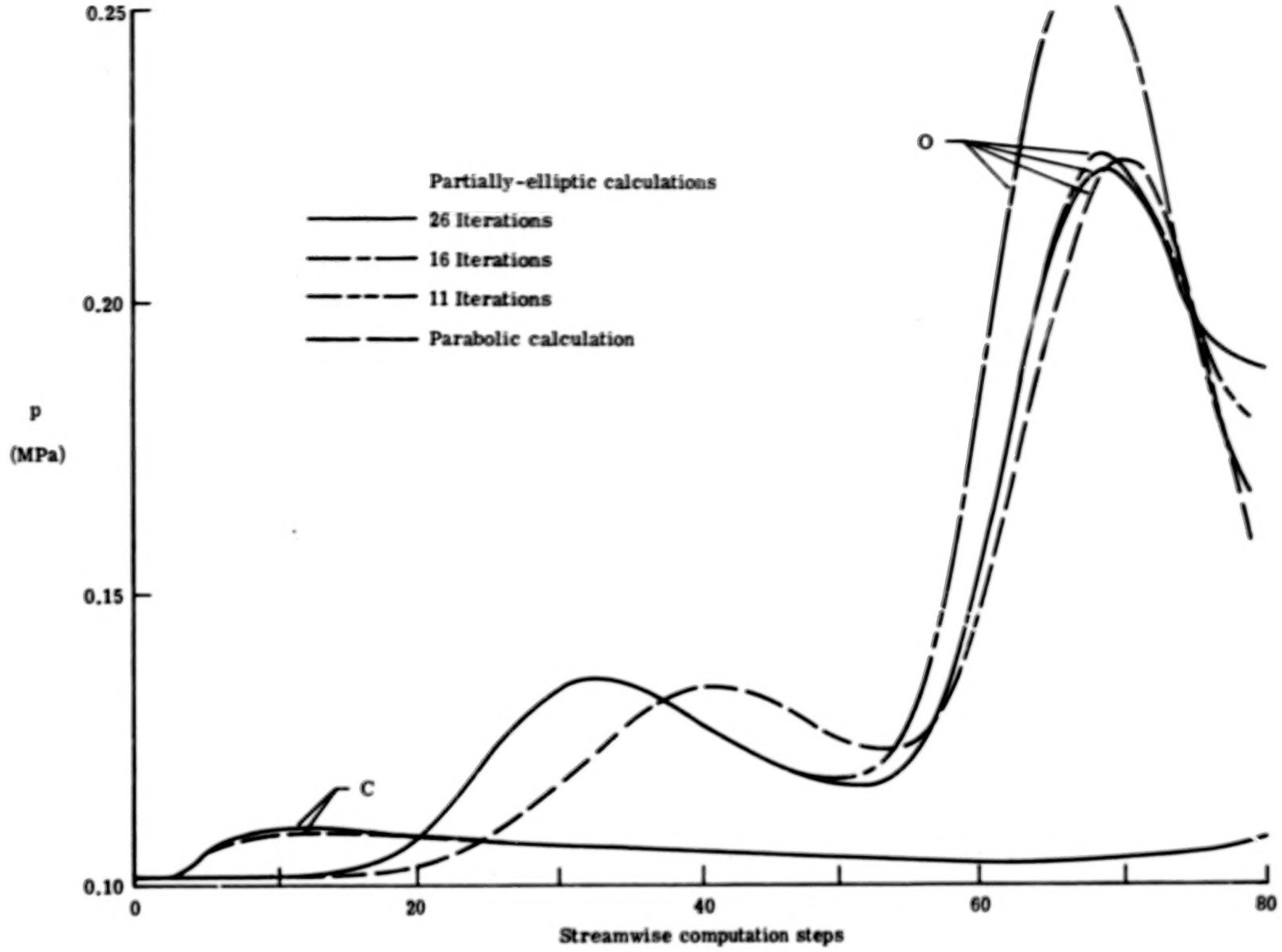


Figure 8.- Convergence behavior of iterative pressure calculation for the reacting case.

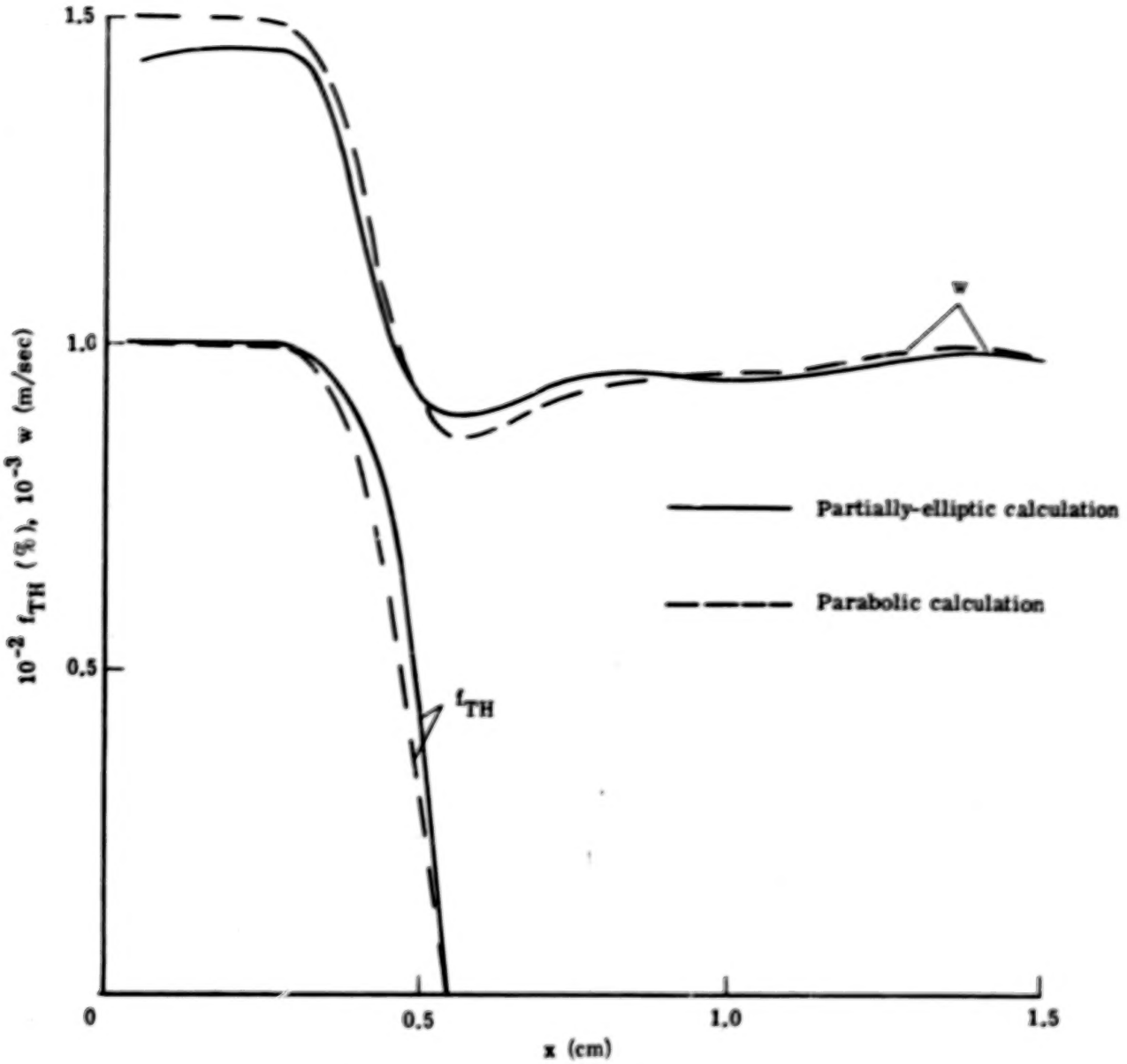
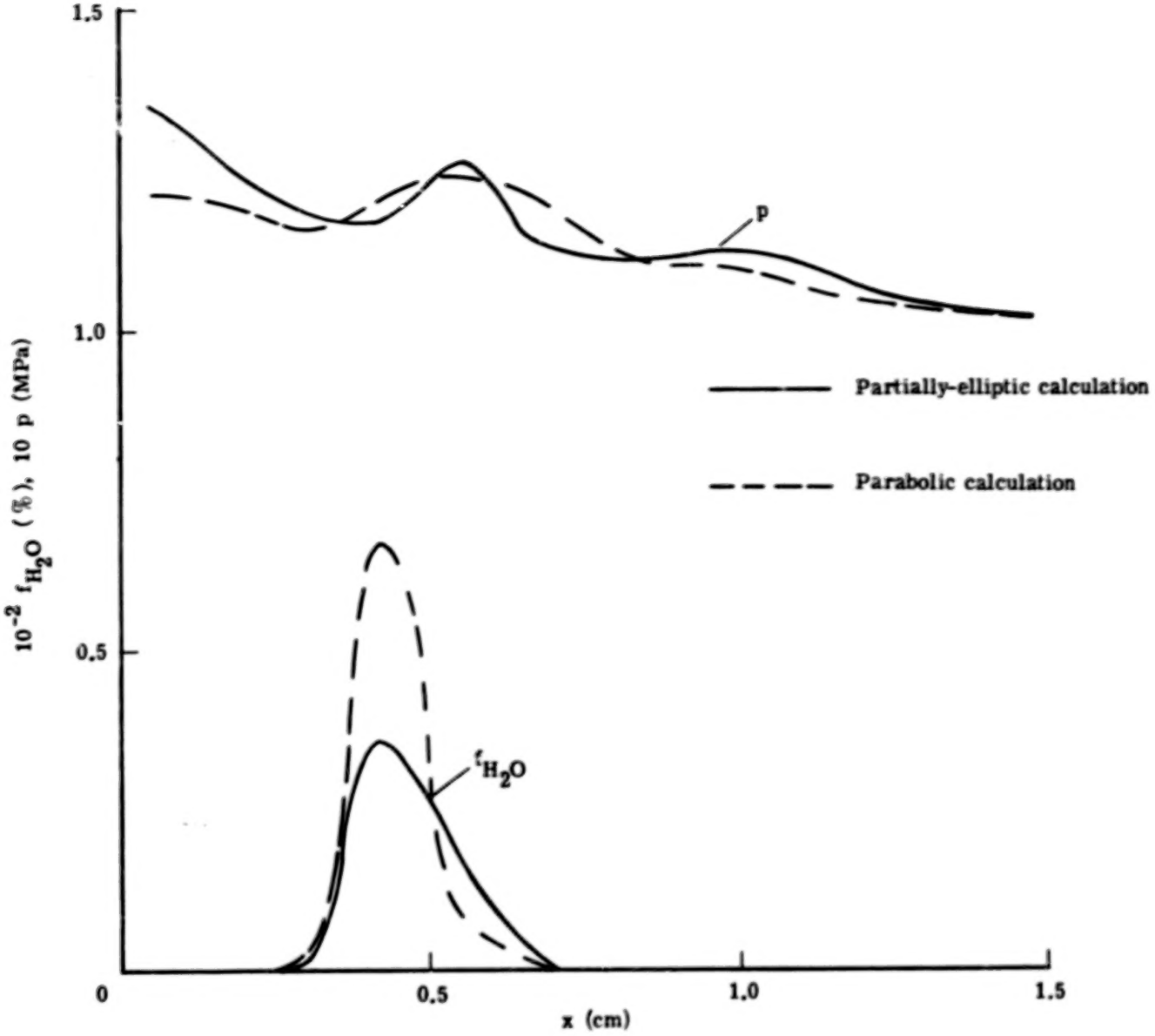


Figure 9.- Cross-duct profiles at the 32nd marching step; y = 0. ,reacting case.

(a) Streamwise velocity and total hydrogen mass fraction.



(b) pressure and water vapor mass fraction

Figure 9.- Concluded.

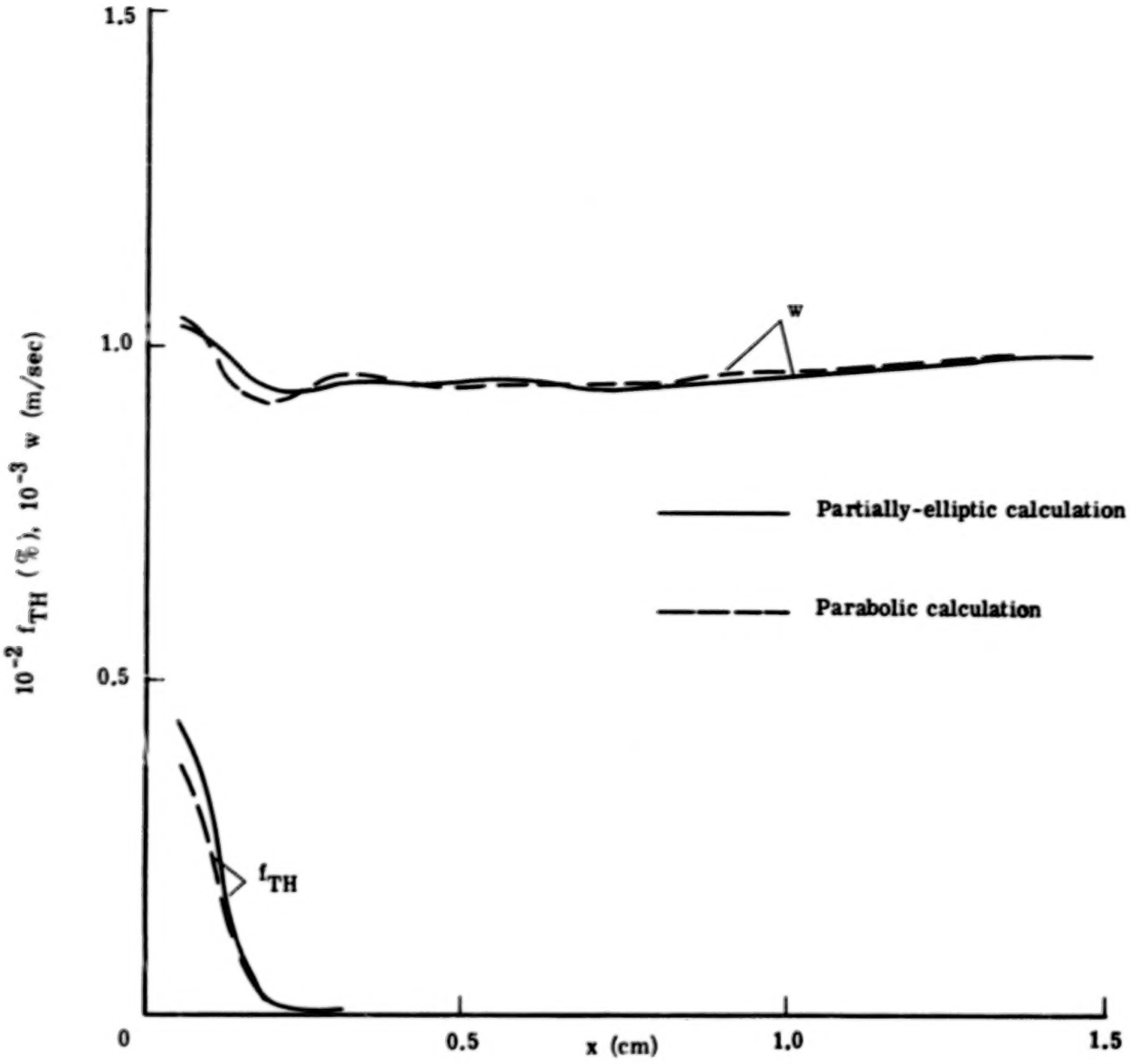
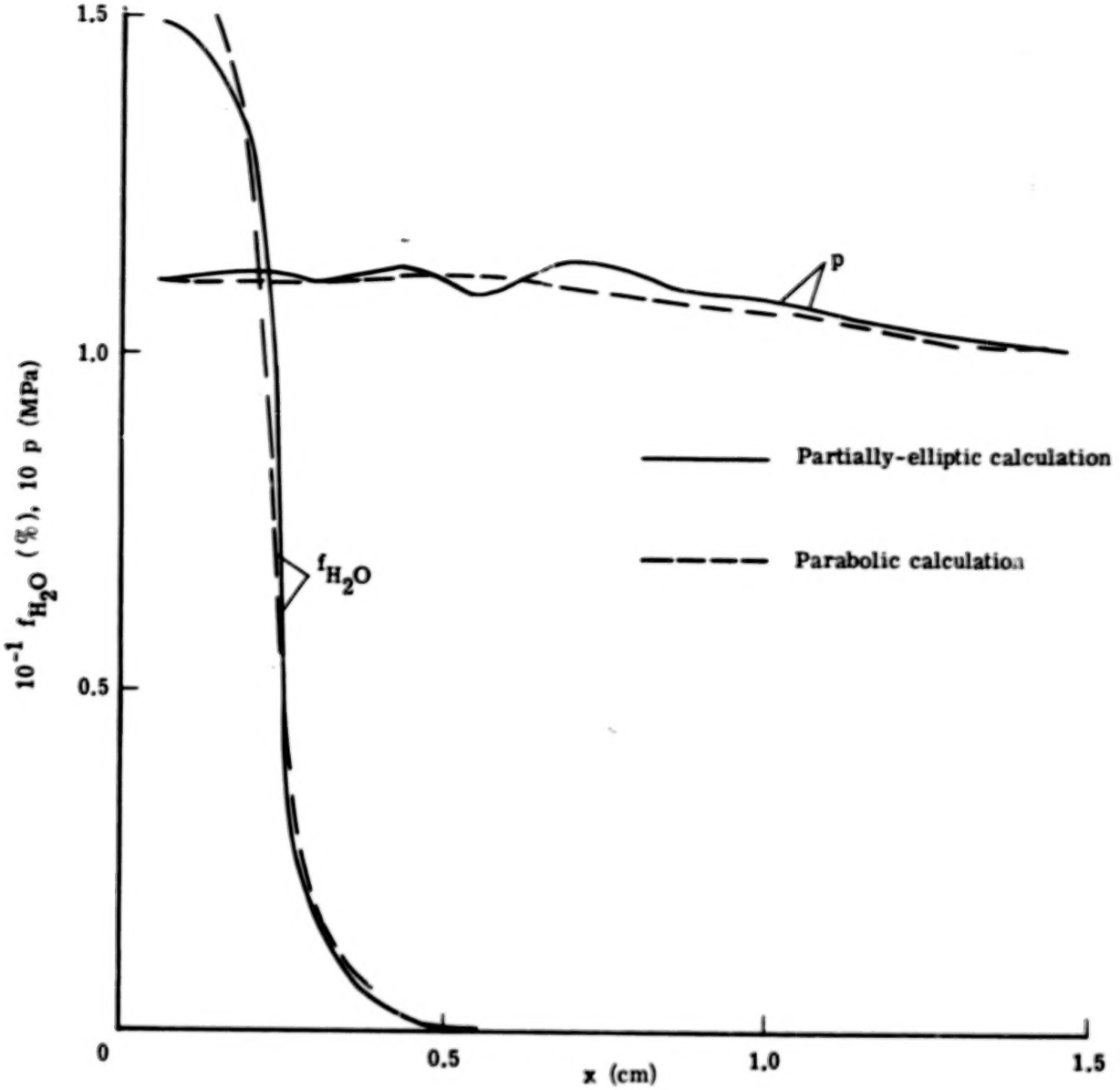


Figure 10.- Cross-duct profiles at the 32nd marching step; y = 0.5 cm ,reacting case.

(a) Streamwise velocity and total hydrogen mass fraction.



(b) Pressure and water vapor mass fraction.

Figure 10.- Concluded.

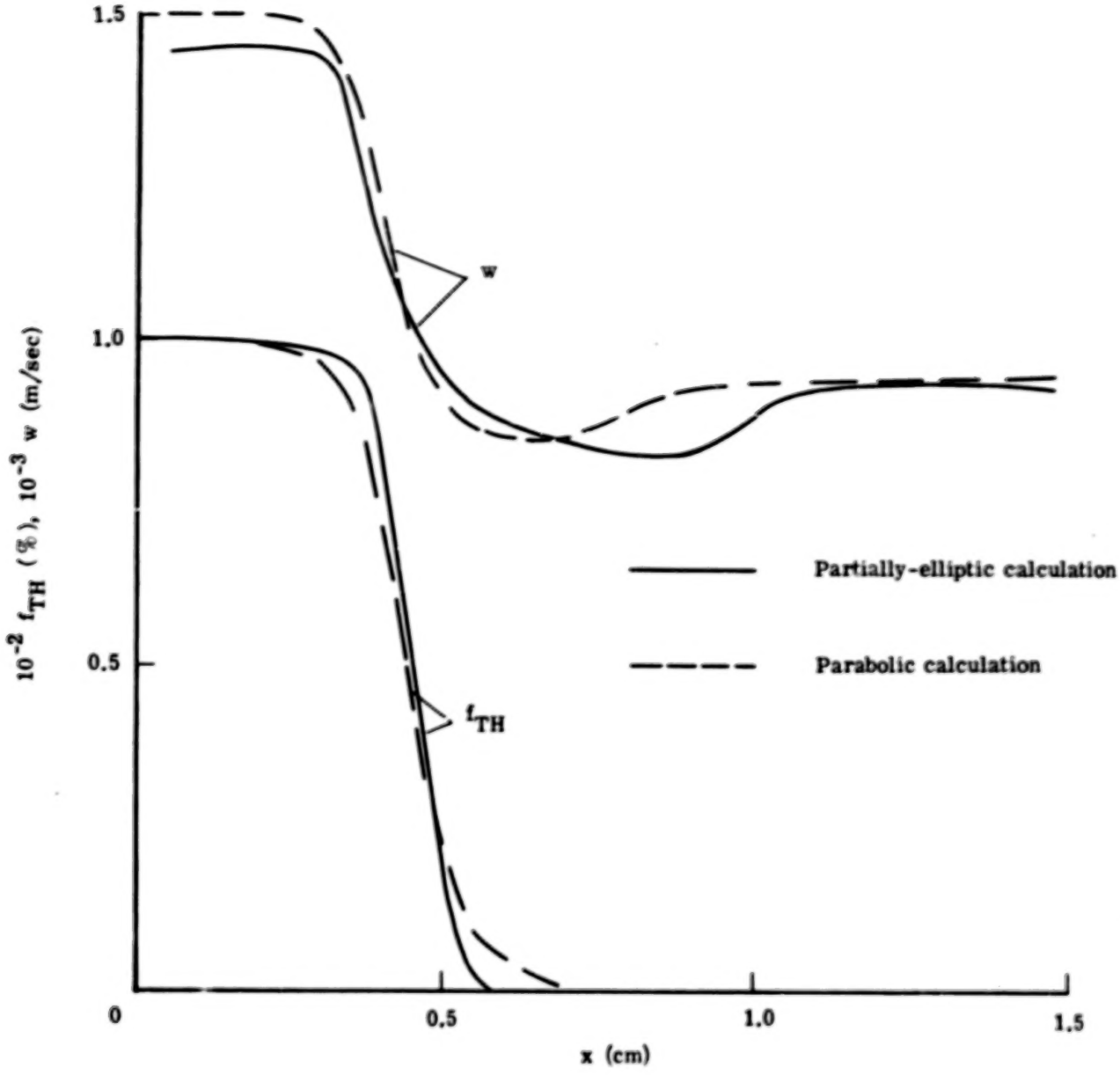
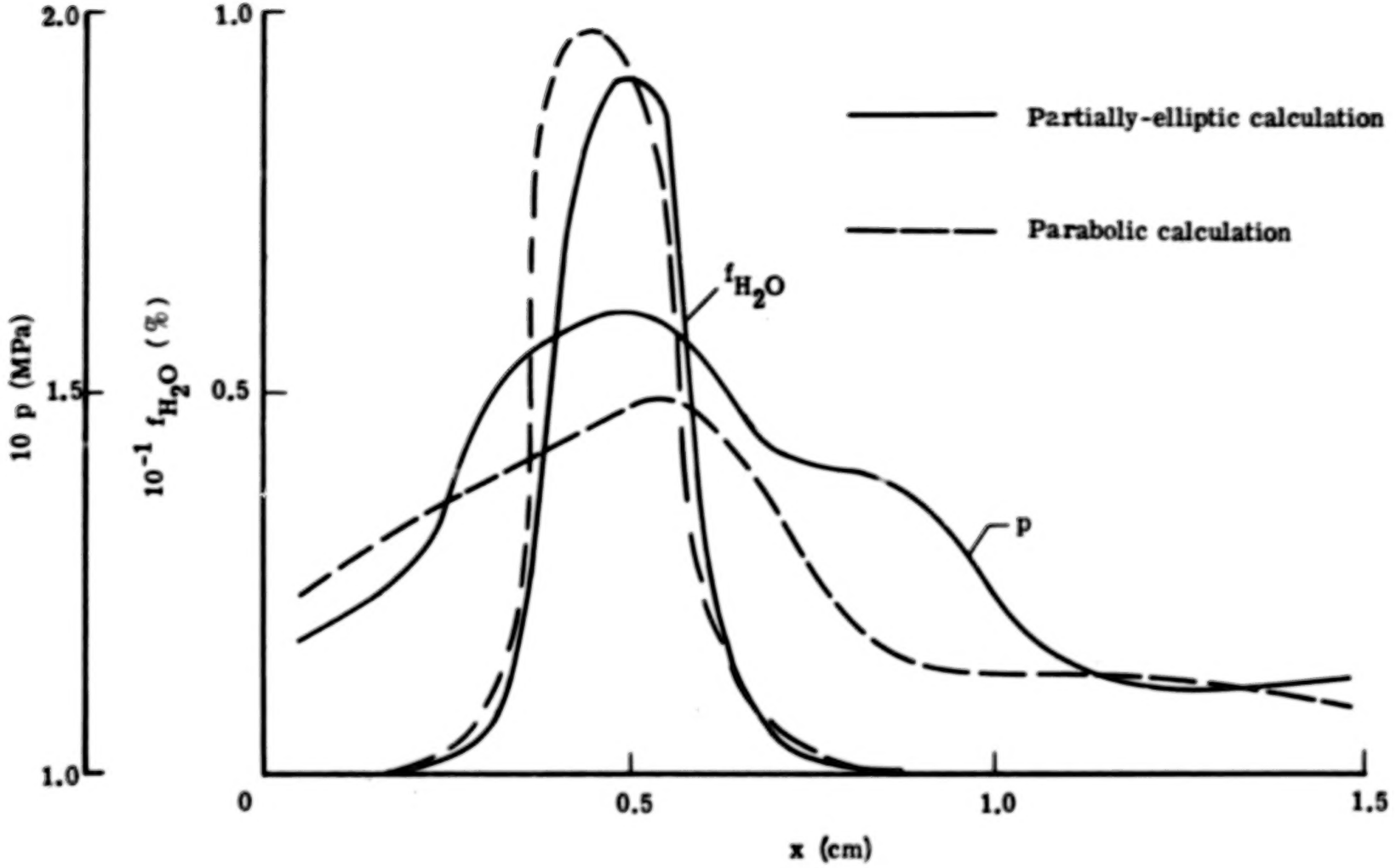


Figure 11.- Cross-duct profiles at the 52nd marching step; y = 0. ,reacting case.

(a) Streamwise velocity and total hydrogen mass fraction.



(b) Pressure and water vapor mass fraction.

Figure 11.- Concluded.

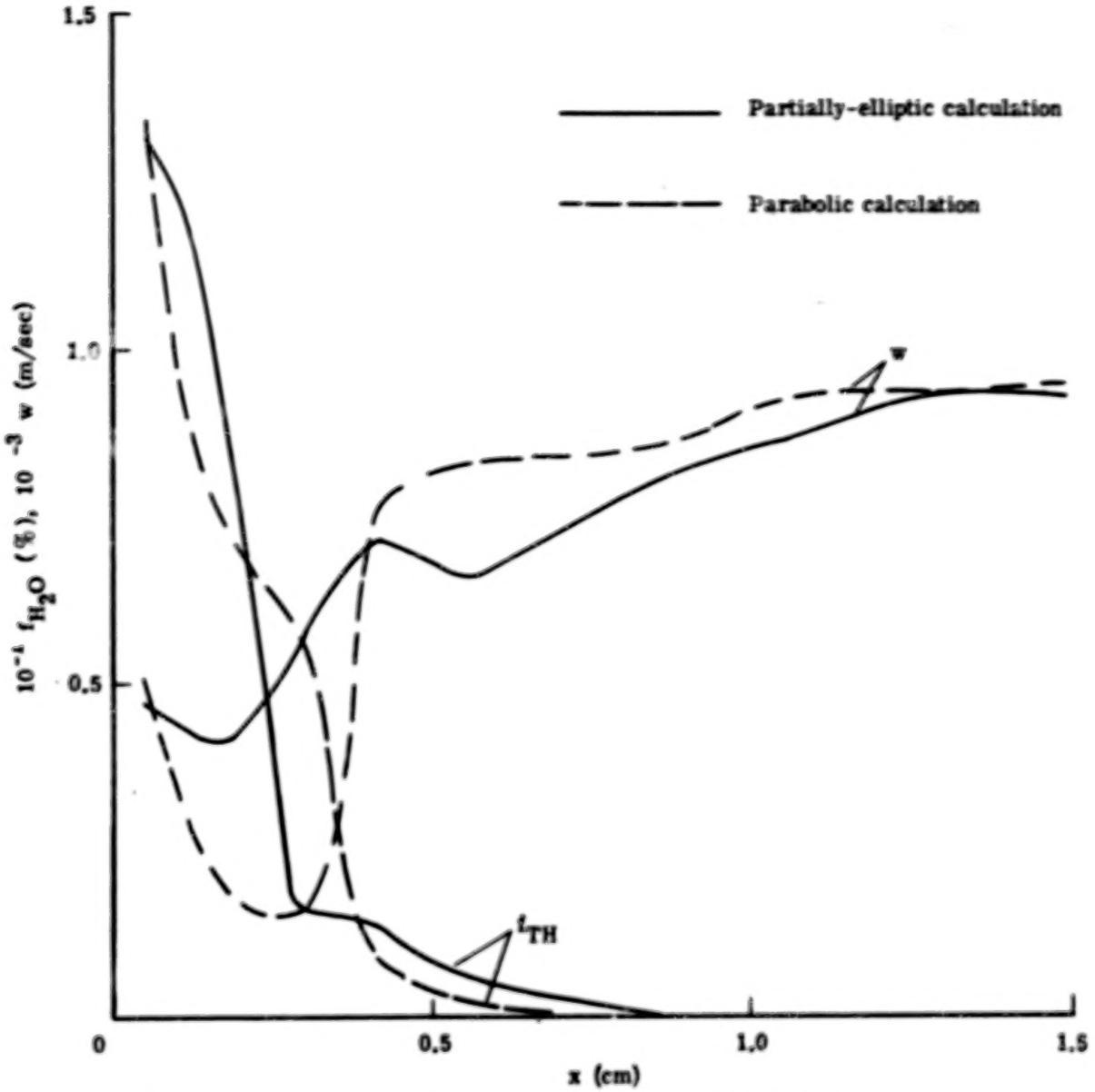
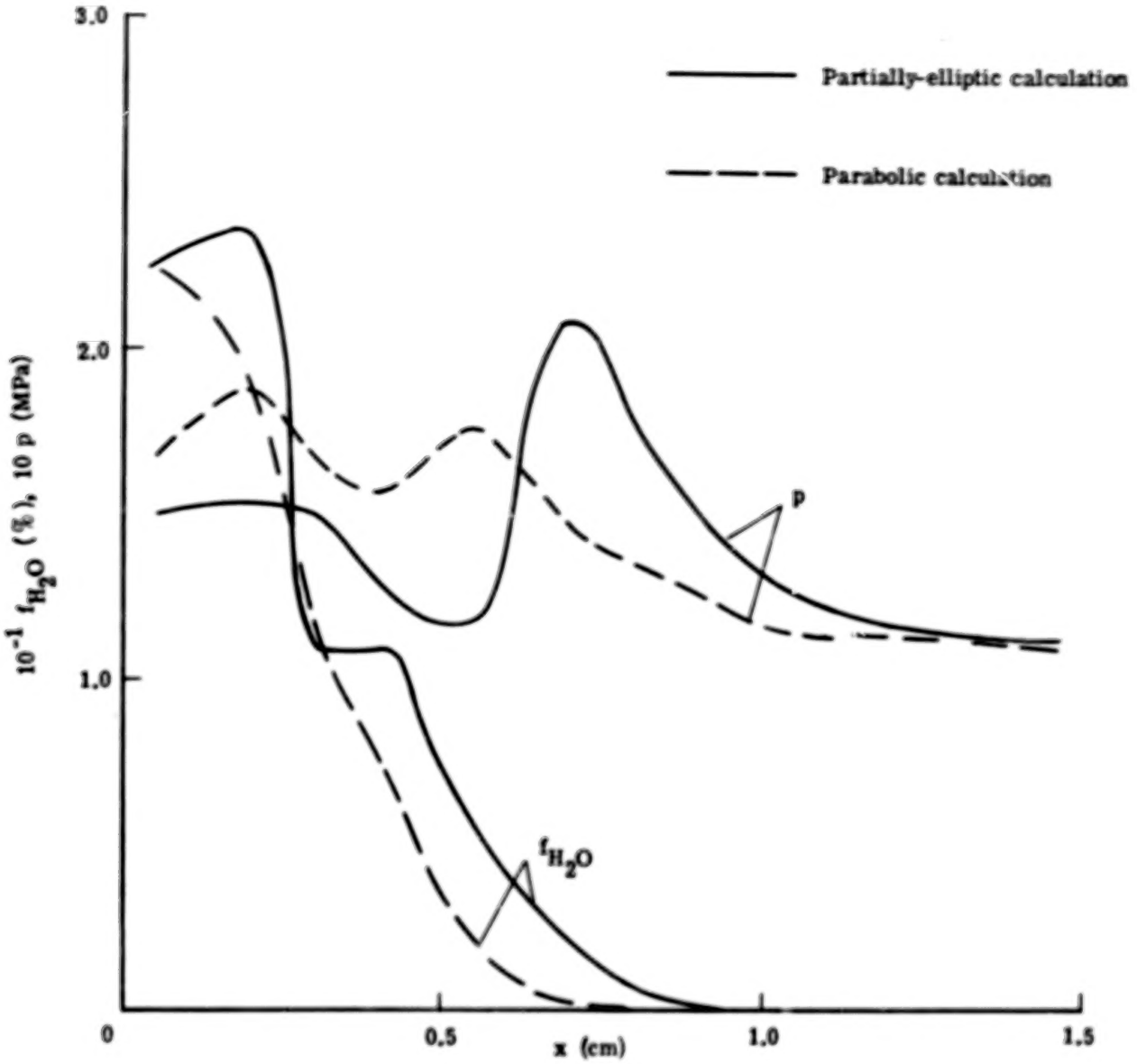


Figure 12.- Cross-duct profiles at the 52nd marching step; y = 0.5 cm ,reacting case.

(a) Streamwise velocity and total hydrogen mass fraction.



(b) Pressure and water vapor mass fraction.

Figure 12.- Concluded.

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Langley technical monitor: John S. Evans

Final Report

16. Abstract

A three-dimensional, partially elliptic, computer program is developed from a concept orginated by Spalding. Without requiring three-dimensional computer storage locations for all flow variables, the partially elliptic program is capable of predicting three-dimensional combustor flow fields with large downstream effects. The program requires only slight increase of computer storage over the parabolic flow program from which it was developed.

A finite-difference formulation for a three-dimensional, fully elliptic, turbulent, reacting, flow field is derived. Because of the negligible diffusion effects in the main flow direction in a supersonic combustor, the set of finite-difference equations can be reduced to a partially elliptic form. Only the pressure field is governed by an elliptic equation and requires three-dimensional storage; all other dependent variables are governed by parabolic equations. A numerical procedure which combines the previously used marching-integration scheme with an iterative scheme for solving the elliptic pressure is adopted.

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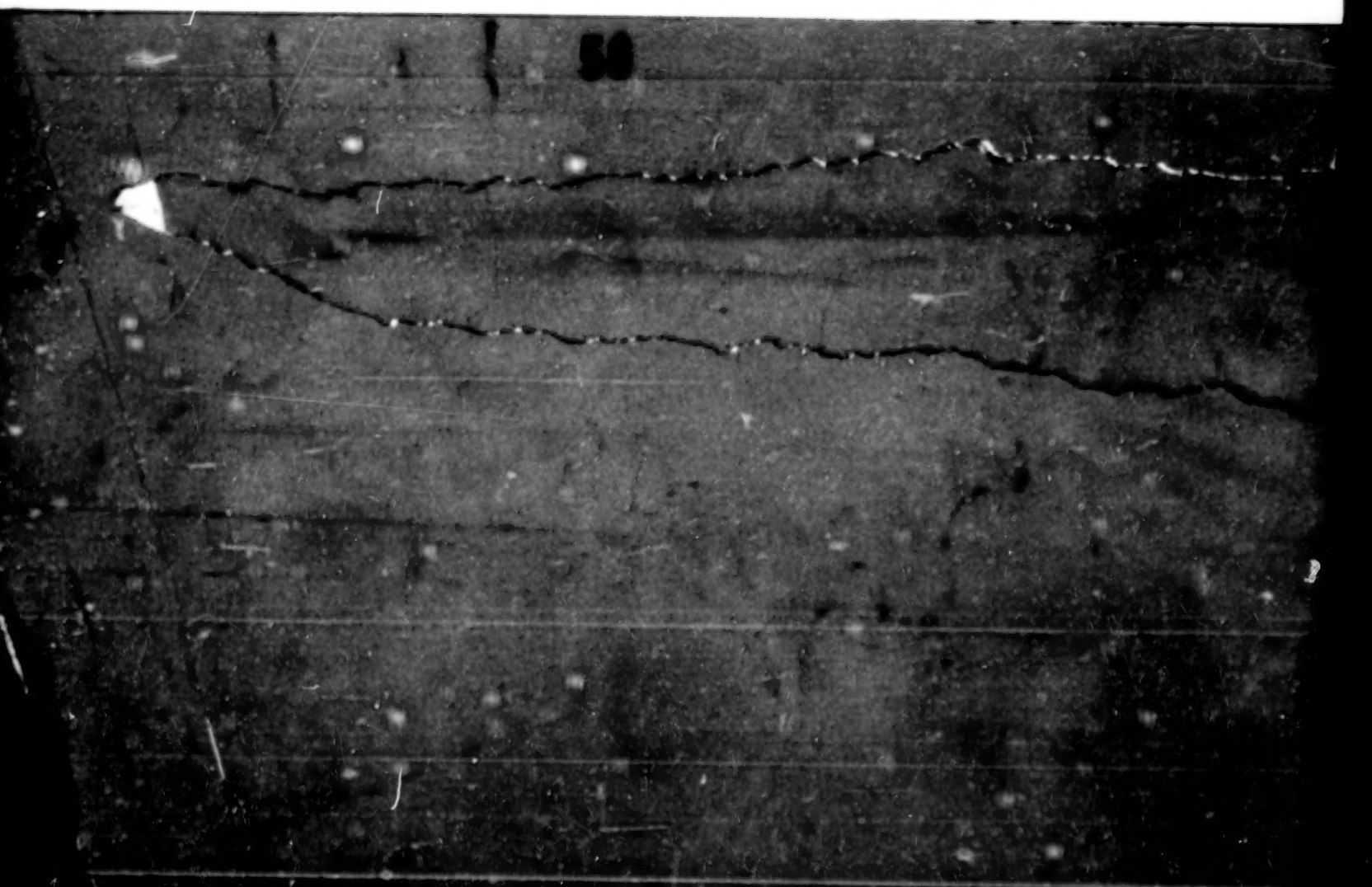
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